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14. ABSTRACT

We have developed a general conceptual-mathematical model is applicable to the fate and advective-dispersive transport of most explosives and its metabolites in the vadose zone or groundwater. The model accounts for the most important physical, chemical and biological processes known or hypothesized to affect the behavior and simultaneous transport of the major explosives (the parent products) such as TNT or RDX, and its various metabolites, as they are being sequentially created by degradation of the parent compound. The parent and daughter compounds are allowed to have different mobilities in the subsurface as dictated by their specific dissolution, sorption and transport properties.

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## Report Title

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## ABSTRACT

We have developed a general conceptual-mathematical model is applicable to the fate and advective-dispersive transport of most explosives and its metabolites in the vadose zone or groundwater. The model accounts for the most important physical, chemical and biological processes known or hypothesized to affect the behavior and simultaneous transport of the major explosives (the parent products) such as TNT or RDX, and its various metabolites, as they are being sequentionally created by degradation of the parent compound. The parent and daughter compounds are allowed to have different mobilities in the subsurface as dictated by their specific dissolution, sorption and transport properties.

To be able to simulate more general conditions than those describe above, we have coupled flow and transport model HYDRUS with a geochemical model PHREEQC. The program can simulate a broad range of low-temperature biogeochemical reactions in water, soil and ground water systems including interactions with minerals, gases, exchangers, and sorption surfaces, based on thermodynamic equilibrium, kinetics, or mixed equilibrium-kinetic reactions.

We have updated the HYDRUS-2D code so that it can consider coupled water, vapor and heat subsurface movements, including a general surface water and energy balance. We have applied the developed model to existing datasets for validation purposes.


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## List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

### (a) Papers published in peer-reviewed journals (N/A for none)

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## (b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

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**Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):** 37

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## Peer-Reviewed Conference Proceeding publications (other than abstracts):

**Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):** 0

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## (d) Manuscripts

Kodešová,R., N. Vignozzi, M. Rohošková, T. Hájková, M. Ko?árek, M. Pagliai, J. Kozák, and J. Šim?nek, Impact of varying soil structure on transport processes in soils, J. Contam. Hydrology, Special Issue "Flow Domains", doi:10.1016/j.jconhyd.2008.10.008, (submitted October 15, 2007; resubmitted March 19, 2008; accepted October 23, 2008), 2008.

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**Number of Manuscripts:** 10.00

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**Number of Inventions:**

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**Graduate Students**

| NAME | PERCENT_SUPPORTED |
|---|---|
| **FTE Equivalent:** | |
| **Total Number:** | |

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## Names of Post Doctorates

| NAME | PERCENT_SUPPORTED |
|---|---|
| Hirotaka Saito | 0.75 |
| Navin Twarakavi | 0.75 |
| Masuru Sakai | 0.40 |
| **FTE Equivalent:** | **1.90** |
| **Total Number:** | **3** |

## Names of Faculty Supported

| NAME | PERCENT_SUPPORTED | National Academy Member |
|---|---|---|
| Jiri Simunek | 0.20 | No |
| **FTE Equivalent:** | **0.20** | |
| **Total Number:** | **1** | |

## Names of Under Graduate students supported

| NAME | PERCENT_SUPPORTED |
|---|---|
| **FTE Equivalent:** | |
| **Total Number:** | |

## Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: ...... 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:...... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale): ...... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering: ...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense ...... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: ...... 0.00

## Names of Personnel receiving masters degrees

| NAME |
|---|
| **Total Number:** |

## Names of personnel receiving PHDs

| NAME |
|---|
| **Total Number:** |

## Names of other research staff

| NAME | PERCENT_SUPPORTED |
|---|---|
| **FTE Equivalent:** | |
| **Total Number:** | |

## Sub Contractors (DD882)

# Inventions (DD882)

# Development of a General Conceptual-numerical Model to Simulate the Fate and Subsurface Transport of Explosives, and the Moisture and Temperature Signatures around Land Mines

## Proposal Number 45690EV

## Final Technical Report

**December 2008**

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## Abstract

We have developed a general conceptual-mathematical model is applicable to the fate and advective-dispersive transport of most explosives and its metabolites in the vadose zone or groundwater. The model accounts for the most important physical, chemical and biological processes known or hypothesized to affect the behavior and simultaneous transport of the major explosives (the parent products) such as TNT or RDX, and its various metabolites, as they are being sequentially created by degradation of the parent compound. The parent and daughter compounds are allowed to have different mobilities in the subsurface as dictated by their specific dissolution, sorption and transport properties.

To be able to simulate more general conditions than those describe above, we have coupled flow and transport model HYDRUS with a geochemical model PHREEQC. The program can simulate a broad range of low-temperature biogeochemical reactions in water, soil and ground water systems including interactions with minerals, gases, exchangers, and sorption surfaces, based on thermodynamic equilibrium, kinetics, or mixed equilibrium-kinetic reactions.

We have updated the HYDRUS-2D code so that it can consider coupled water, vapor and heat subsurface movements, including a general surface water and energy balance. We have applied the developed model to existing datasets for validation purposes.

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# Objectives

This project seeks to develop a general conceptual-numerical model to predict the fate and subsurface transport of explosives, and moisture and temperature signatures around land mines. The primary aims of the project are to:

- Develop a general process-based mathematical model describing the fate and transport of explosives and energetics in variably-saturated soil and groundwater systems.

- Develop a coupled model for water, vapor, and heat movement in the subsurface, including a surface water and energy balance module.

- Develop efficient numerical solutions and associated software of the resulting process-based model.

- Use the model to analyze existing data sets on the behavior and transport of explosives.

- Evaluate the effects of previously ignored coupled water, vapor, and heat transport processes on moisture and temperature signatures around land mines.

# Approach

Current modeling of the fate and transport of major explosives is mostly carried out using either Modflow combined with MT3D for groundwater systems, or FEMWATER for vadose zone type investigations. Neither of these codes accounts for all major processes involved in the fate and subsurface transport of explosives and their metabolites, such as nonlinear and kinetic dissolution and sorption, simultaneous transport of multiple metabolites, simultaneous transport in both the liquid and vapor phase, and temperature dependence of transport and reaction parameters. We were following two approaches to overcome this problem:

- *Modifying HYDRUS models* – We have developed a general conceptual-mathematical model is applicable to the fate and advective-dispersive transport of most explosives and its metabolites in the vadose zone or groundwater. The model accounts for the most important physical, chemical and biological processes known or hypothesized to affect the behavior and simultaneous transport of the major explosives (the parent products) such as TNT or RDX, and its various metabolites (the daughter products) such as 2ADNT, 2,4DANT, 1,3,5TNB, as they are being sequentionally created by degradation of the parent compound. The parent and daughter compounds are allowed to have different mobilities in the subsurface as dictated by their specific dissolution, sorption and transport properties. In its most general case, the model permits contaminants to reside in all three phases, i.e., in the liquid, solid (precipitated and sorbed), and gaseous phases.

- *Coupling flow and transport model HYDRUS with a geochemical model PHREEQC* – To be able to simulate more general conditions than those describe above, we have coupled flow and transport model HYDRUS with a geochemical model PHREEQC (developed by USGS). PHREEQC The program can simulate a broad range of low-temperature biogeochemical reactions in water, soil and ground water systems including interactions with minerals, gases, exchangers, and sorption surfaces, based on thermodynamic equilibrium, kinetics, or mixed equilibrium-kinetic reactions. This coupled program tremendously increases applicability of HYDRUS, that by itself numerically solves the Richards equation for variably-saturated water flow and advection-dispersion type equations for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers transport due to conduction and convection with flowing water. The solute transport equations consider advective-dispersive transport in the liquid phase.

Closely related to the presence of explosives and energetics in the environment is the presence of buried land mines. Field studies and numerical simulations may be used to study how land mines influences water content and temperature profiles around the land mines and whether these altered moisture and temperature signatures could be used for land mine detection. Existing studies did not consider all of the processes that may be important for developing moisture and temperature signatures of buried land mines, especially in extreme (tropical, arid) climates. However, the complex interactions of water, vapor, and heat movement cannot be studied without a model that considers these strongly coupled interactions, including boundary conditions calculated from a surface water and energy balance. To overcome this problem we have:

- Updated the HYDRUS-2D code so that it can consider *coupled water, vapor and heat subsurface movements, including a general surface water and energy balance* (thorough mathematical description of the model that is being implemented is presented in the proposal).

- *Developed efficient numerical solutions and associated software of the resulting process-based mode*. Efficient and stable solutions of the coupled water, vapor and heat subsurface movement, additionally coupled with water and energy balance (which are all mutually dependent on each other) requires advanced numerical techniques. We have developed several stability criteria that stabilize the numerical solution.

- *Applied developed model to existing datasets for validation purposes*. For this purpose we are using a dataset that was developed by Binayak Mohanty at the field site near the University of California Agricultural Experimental Station in Riverside, California, during the fall of 1995 and that involves field soil temperature and water content data collected at different depths.

## Significance and Army Value

Concern is increasing about the presence of explosives and energetics in the subsurface environment. Such chemicals are the result of the manufacture, distribution, testing and/or unsafe disposal of ammunition. They often leach through the vadose zone into groundwater and thus threaten underlying or down-gradient water resources. Current modeling of the fate and transport of major explosives is mostly carried out using either Modflow (combined with MT3D) for groundwater systems, or FEMWATER for vadose zone type investigations. None of these codes accounts for all major processes involved in the fate and subsurface transport of explosives and their metabolites, such as nonlinear and kinetic dissolution and sorption, simultaneous transport of multiple metabolites, simultaneous transport in both the liquid and vapor phase, and temperature dependence of transport and reaction parameters. We have implemented all of these processes in the HYDRUS computer software packages. The proposed conceptual-mathematical model is the first of its kind to account for the full range of processes and subsurface flow/transport properties known to affect the fate and transport of explosives and its metabolites in the vadose zone. The model permit scientists, engineers and other users to tackle a variety of subsurface (especially vadose zone) flow and transport problems that cannot be addressed with existing tools. The updated HYDRUS-1D model has been released to the public domain and is currently being downloaded during a single month by up to 250 scientists, students, and other users from around the world.

One problem closely related to the presence of explosives and energetics in the environment is the presence of land mines. New censors for land mine detection are now actively being sought. Field studies and numerical simulations can be used to study how land mines influence water content and temperature profiles in soils around the land mines, and whether these altered moisture and temperature signatures can be used for land mine detection. Previous numerical studies carried out using HYDRUS-2D did not consider all processes that are important for development of such signatures, especially in relatively extreme (tropical, arid) climates, i.e., coupled water, vapor and heat movement in the subsurface, and coupled surface water dynamics and the energy balance. The updated model is now able to fully describe complex coupled processes in the near surface environment in which buried land mines are typically installed. The model thus allows users to make more precise predictions of the moisture and temperature signatures around buried land mines.

## Accomplishments

During this 4-year project, the following tasks have been completed:

- We have implemented in the HYDRUS-1D code the coupled movement of water, vapor, and heat in the subsurface, as well as interactions of these subsurface processes with the mass and energy balance at the soil surface. The code considers the movement of liquid water and water vapor in the subsurface to be driven by both pressure head (isothermal transport) and temperature (thermal transport) gradients. The heat transport module considers movement of soil heat by conduction, convection of sensible heat by water flow, transfer of latent heat by diffusion of water vapor, and transfer of sensible heat by diffusion of water vapor. Water flow and heat transport are coupled not only in the subsurface but also by the surface boundary water and energy balance. The developed code allows a very flexible way of using various types of meteorological information at the soil-atmosphere interface for evaluating surface water and energy balance.

- The coupled model was evaluated using field soil temperature and water content data collected at different depths at the field site near the University of California Agricultural Experimental Station in Riverside, California, during the fall of 1995. We demonstrated the use of standard daily meteorological variables in simulating continuous changes in water contents, temperatures, and water, vapor, and heat fluxes. The meteorological data were collected from a nearby weather station and used to predict temporal net radiation changes. Soil temperatures and water contents in three different depths (2, 7, and 12 cm) were simulated using the measured soil hydraulic properties, estimated thermal properties, applied irrigation fluxes, and estimated net radiations over a period of 15 days. Simulated temperatures and water contents were in good agreement with measured values. Simulation results also revealed that heat transport was strongly associated with vapor transport.

- A new coupled model for multicomponent reactive transport during transient variably-saturated flow HP1 was developed. The model combines two comprehensive existing models: HYDRUS-1D and PHREEQC. HYDRUS-1D is a one-dimensional finite element model simulating the movement of water, heat and multiple solutes in variably-saturated heterogeneous or layered soils subject to a variety of atmospheric and other boundary conditions. PHREEQC is a computer program simulating the behavior of complex chemical systems, including such reactions as speciation, ion exchange, surface complexation, and mineral precipitation/dissolution.

- The versatility of HP1 was illustrated by means of simulating the transport of TNT and its degradation products. TNT (the parent product) was assumed to be initially present in the top 5 cm of the soil, and dissolving at a certain rate. When dissolved, TNT was assumed to degrade to form the daughter products 2ADNT and 4ADNT, which further degrade to form the final daughter product TAT. Different distribution coefficients for linear sorption were assumed for TNT, 2ADNT, 4ADNT, and TAT, respectively. Because of less sorption, TAT moved fastest through the soil profile, with TNT second fastest, and 2ADNT and 4ADNT at similar velocities. This simulation demonstrated that ground water may be more vulnerable to leaching of TNT daughter products (notably TAT) than of the parent compound itself, and that sensors detecting daughter products may provide an early warning of possible TNT leaching. The model can, however, be used to a large number of other applications involving both physical transport and various chemical reactions.

- To examine surface temperature evolution, a soil heat and water transfer model (HYDRUS-1D) has been coupled to an atmospheric surface layer scheme. Idealized simulations have been carried out for different soils, initial soil moisture conditions, and atmospheric flow properties (stability, surface shear stress). From the simulation results, the coupling between soil properties, surface temperature, and sensible heat flux has been examined.

- A new package, called HYDRUS, has been developed for the groundwater flow model MODFLOW (Harbaugh et al., 2000) to represent the effects of vadose zone processes in this widely used groundwater flow model. Being fully incorporated into the MODFLOW program, the HYDRUS package provides MODFLOW with recharge fluxes at the water table, while MODFLOW provides HYDRUS with the position of the groundwater table that is used as the bottom boundary condition in the package. Twarakavi et al. (2008) compared the HYDRUS package to other contemporary modeling approaches and evaluated its performance for three case studies of increasing complexity. The HYDRUS package provided a much more efficient alternative and could account better for vadose zone processes than other existing MODFLOW packages. For large-scale ground water problems, the HYDRUS package provides an optimal trade-off between computational effort and accuracy of model simulations for coupled vadose zone – groundwater problems.

- For the collaborative project between Prof. Simunek and researchers from US Army Corps of Engineers, Engineer Research and Development Center Waterways Experiment Station, Environmental Laboratory, Vicksburg, MS (Drs. Katerina M. Dontsova and Judy C. Pennington), we have modified the HYDRUS-1D software package a) to allow dissolution of composition B during certain time, b) to specify maximum allowed concentration in the liquid phase due to dissolution, c) to assign the same degradation rates to solid and liquid phases, d) to allow simulation of the transport of two daughter products, e) to redefine the objective function of the inverse problem to accommodate our experimental data, i.e., to sum up concentrations when C14 labeling was used and to use daughter product's concentrations in the objective function.

- We have applied the previously updated HYDRUS-1D code that is intended to simulate the fate and transport of explosives and their metabolites in the subsurface to laboratory columns studies involving the transport of TNT, RDX (hexahydro-1,3,5- trinitro-1,3,5-triazine), HMX, and the explosive formulation, Composition B, in solid and dissolved forms under saturated and unsaturated conditions. Experiments were carried out at two different soils and flow interruption technique was employed to determine if soils were at equilibrium with solution. The analyses demonstrates that adsorption coefficients determined from the column experiment were different from ones determined in batch tests for the same soils, indicating that values determined from batch isotherms may not be adequate to predict fate of RDX and TNT in the soils. A possible explanation for the difference between $K_d$ values predicted by the model and those obtained from the batch studies is that batch studies combine reversible and irreversible sorption into one single coefficient $K_d$, while model allows to separate processes of reversible and irreversible sorption.

## Technology Transfer to Army Scientists

- On November 24, 2004, Prof. Simunek visited with Drs. Katerina M. Dontsova and Judy C. Pennington from US Army Corps of Engineers, Engineer Research and Development Center Waterways Experiment Station, Environmental Laboratory, Vicksburg, MS and discussed planned column studies design to study transport of explosives in porous materials. Applicability of the numerical model HYDRUS-1D developed by Prof. Simunek to analyze experimental data was also discussed.

- During this first year we have closely collaborated with Katerina M. Dontsova and Judy C. Pennington from US Army Corps of Engineers, Engineer Research and Development Center Waterways Experiment Station, Environmental Laboratory, 3909 Halls Ferry Road, Vicksburg, MS 39180. We have provided support in analyzing column experiment involving saturated water flow and dissolved explosives (TNT, RDX, HMX). Nonequilibrium processes were experimentally analyzed using flow interruption. The numerical analyses was carried out using HYDRUS-1D, numerical model develop by our research group. We have made several modification allowing simultaneous analyses of the parent compound as well as its daughter products (which is one of the goal of our project).

- Dr. Katerina M. Dontsova participated in the short course presented by Prof. Simunek entitled "Advanced Modeling of Water Flow and Solute Transport in the Vadose Zone", organized by the Dept. of Agronomy and Soils Auburn University Auburn, Alabama, April 1-2, 2005.

- Prof. Simunek collaborated on a proposal "Pathways and mechanisms of sorption and vadose transport of high explosives". Proposal was written by Dr. Judith Pennington (ERDC-EL), Katerina Dontsova (University of Mississippi), Jiri Simunek (University of California, Riverside), and John K. Newman (ERDC-GSL) for The Engineer Research and Development Center, Basic Research (6.1) Program. The proposal received funding and is currently being carried out. Numerical models developed in the ARO-funded research are used in this project.

- On July 26, 2006, Prof. Simunek visited with Drs. Katerina M. Dontsova and Judy C. Pennington from US Army Corps of Engineers, Engineer Research and Development Center Waterways Experiment Station, Environmental Laboratory, Vicksburg, MS and discussed mutual collaboration on analyses of column studies design to study transport of explosives in unsaturated porous materials. Applicability of the numerical model HYDRUS-1D developed by Prof. Simunek to analyze experimental data was also discussed. Possibility to further extend the project to account for the colloid-facilitated transport of explosives was discussed.

- Collaboration has been established between Prof. Simunek and the group led by Dr. Ingrid Padilla from the Department of Civil Engineering, University of Puerto Rico

Mayaguez, Puerto Rico. Dr. Ingrid Padilla is studying the transport of explosives in shallow soils under variable environmental conditions and is receiving MURI funding.

- Prof. Simunek was teaching a short course on "The advanced modeling of water flow and solute transport in variably-saturated media with the HYDRUS software" at the Department of Civil Engineering, University of Puerto Rico Mayaguez, Puerto Rico from October 31 to November 3, 2006. During this workshop, Dr. Simunek was teaching how to use numerical tools developed using funding from this project. The workshop was offered to the group led by Dr. Ingrid Padilla, who is studying the transport of explosives in shallow soils under variable environmental conditions and who receives MURI funding. The short course provided a unique opportunity to transfer technology (mostly theoretical) developed in one ARO project to the MURI funded applied project. ARO provided supplemental funding to the cover traveling costs, lodging, and per-diem for the short course instructor Dr. Simunek.

- Prof. Simunek closely collaborated with Katerina M. Dontsova and Judy C. Pennington from US Army Corps of Engineers, Engineer Research and Development Center Waterways Experiment Station, Environmental Laboratory, 3909 Halls Ferry Road, Vicksburg, MS 39180. We have provided support in analyzing column experiment involving saturated water flow and dissolved explosives (TNT, RDX, HMX). Nonequilibrium processes were experimentally analyzed using flow interruption. The numerical analyses was carried out using HYDRUS-1D, numerical model develop by our research group. We have made several modification allowing simultaneous analyses of the parent compound as well as its daughter products (which is one of the goal of our project).

- Results of this collaboration appeared in the following research report "Dontsova, K. M., M. Chappell, J. Šimůnek, and J. C. Pennington. Dissolution and transport of nitroglycerin, nitroguanidine and ethyl centralite from M9 and M30 propellants in soils. *In* Characterization and fate of gun and rocket propellant residues on testing and training ranges: Final report. ERDC TR-08-xx. U.S. Army Engineer Research and Development Center, Vicksburg, MS (in print)" and reported at the Soil Science Society of America annual meeting in Dontsova, K., J. Šimůnek, J. Pennington, and C. Price, Facilitated transport of high explosives in mineral soils, Soil Science Society America annual meeting, *Agronomy Abstracts*, published on a CD-ROM as abstract 283-9, ASA, Madison, 2007.

- Prof. Simunek collaborated on a proposal "Pathways and mechanisms of sorption and vadose transport of high explosives". Proposal was written by Dr. Judith Pennington (ERDC-EL), Katerina Dontsova (University of Mississippi), Jiri Simunek (University of California, Riverside), and John K. Newman (ERDC-GSL) for The Engineer Research and Development Center, Basic Research (6.1) Program. The proposal received funding and is currently being carried out. Numerical models developed in the ARO-funded research are used in this project.

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## Research Reports (with other scientists funded by the Army)

- Dontsova, K. M., M. Chappell, J. Šimůnek, and J. C. Pennington. Dissolution and transport of nitroglycerin, nitroguanidine and ethyl centralite from M9 and M30 propellants in soils. *In* Characterization and fate of gun and rocket propellant residues on testing and training ranges: Final report. ERDC TR-08-xx. U.S. Army Engineer Research and Development Center, Vicksburg, MS (in print).

# Awards

Don and Betty Kirkham Award (awarded by the Soil Science Society of America for a mid career scientist who has made outstanding scholarly achievements and educational contributions in soil physics), 2005.

CRCIF (Cooperative Research Center Irrigation Futures, Australia) Visiting Fellow, 2007.

Fellowship from the Japan Society for the Promotion of Science, Tokyo, Japan, June 21 – July 5, 2008.

“Distinguished Visitor” of the Blaustein Center for Scientific Cooperation of the Sede Boqer Campus, for 2009.

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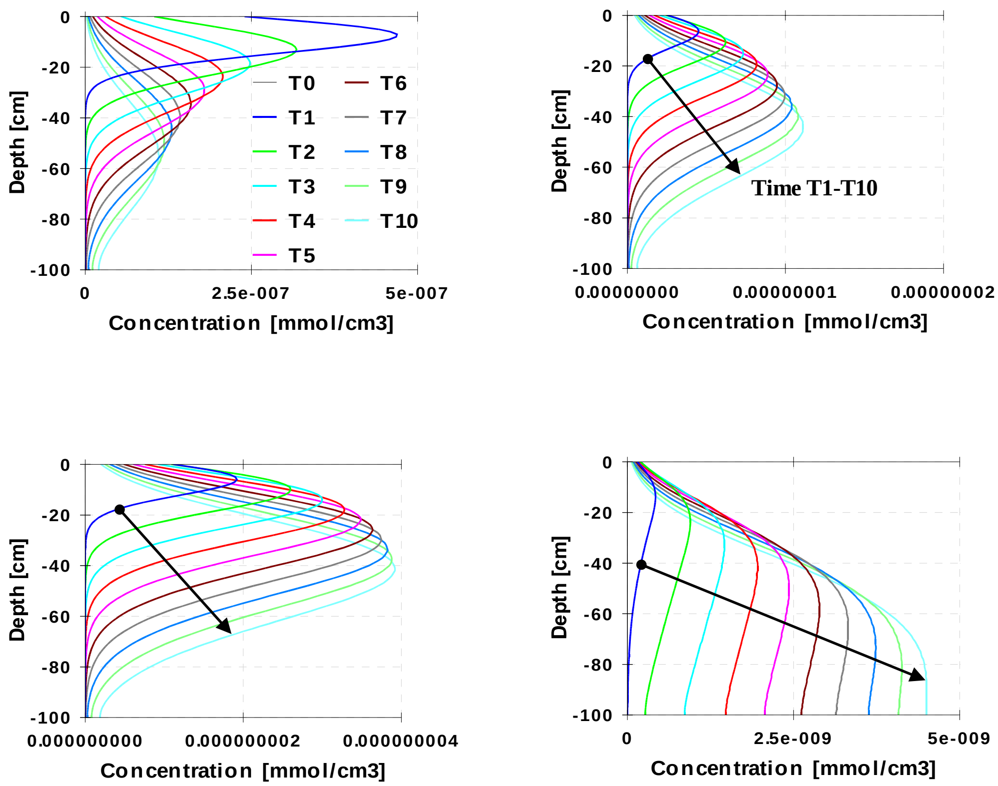


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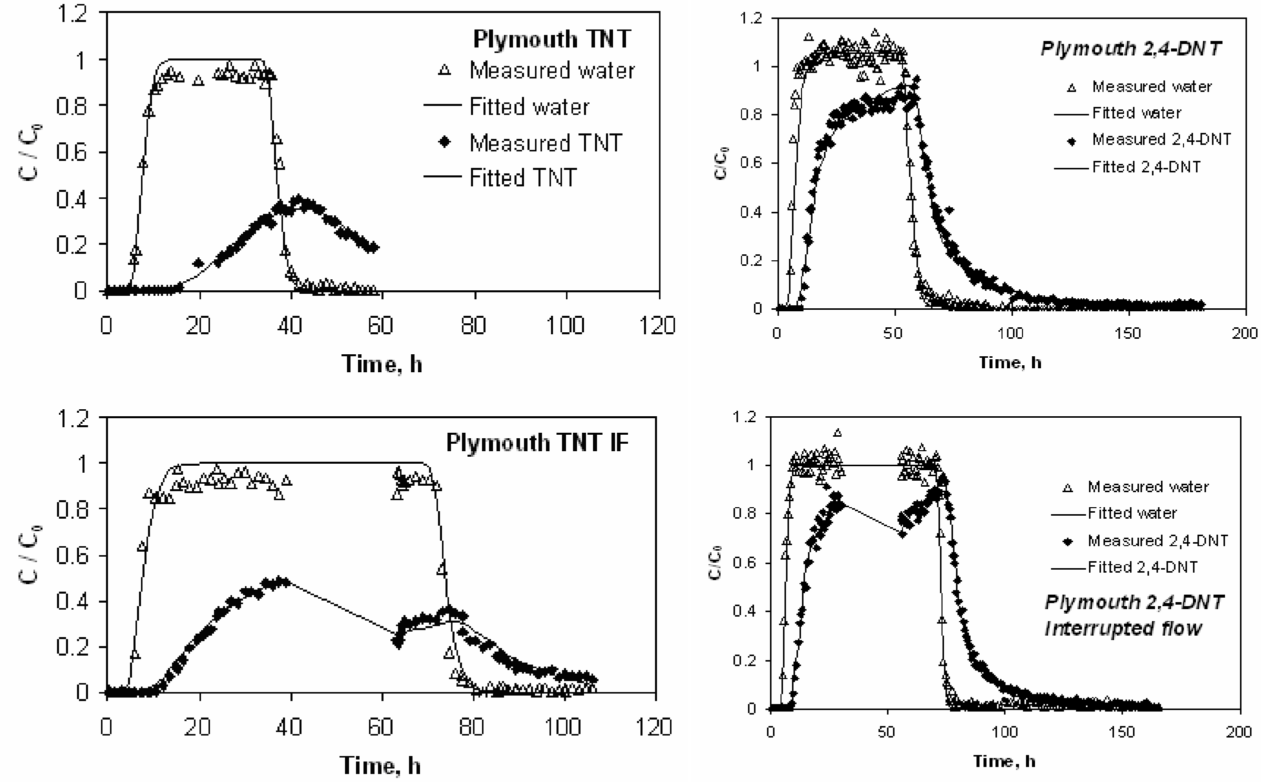


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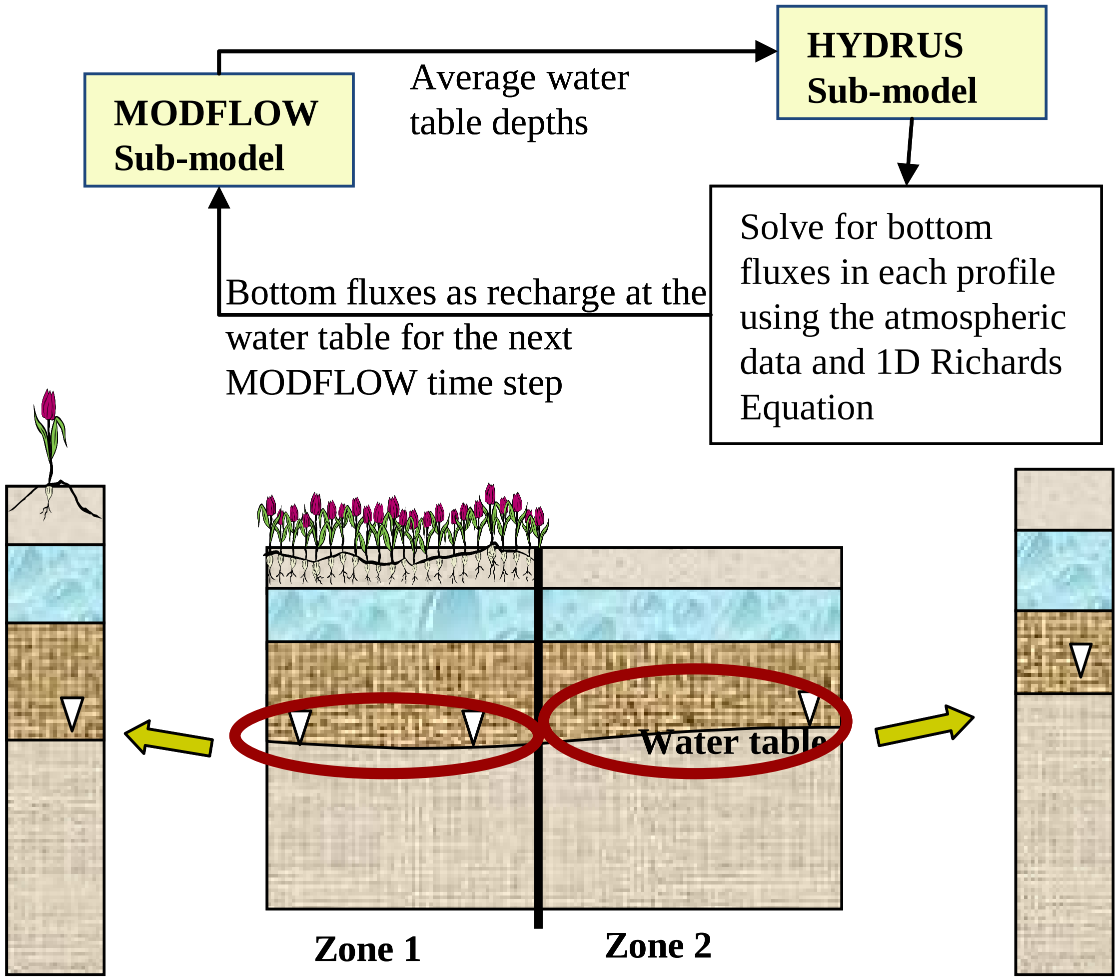


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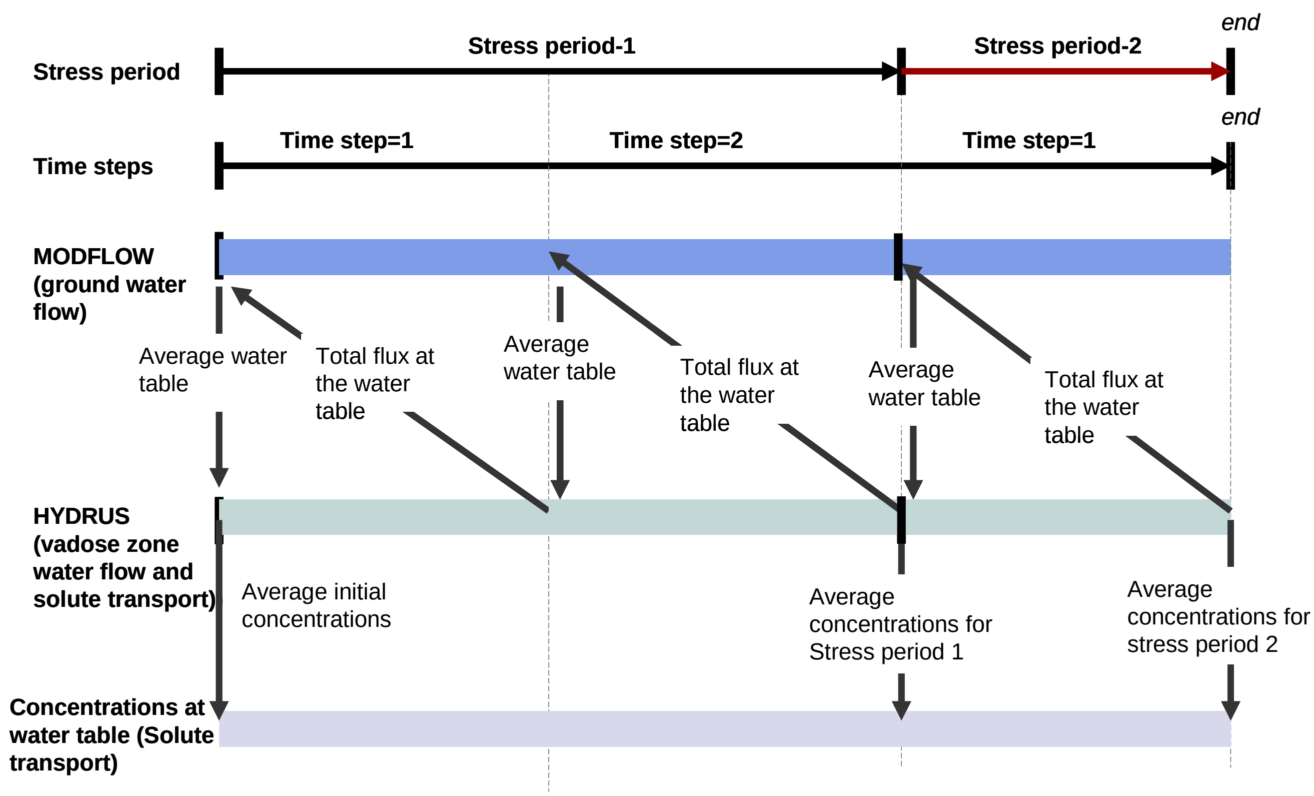


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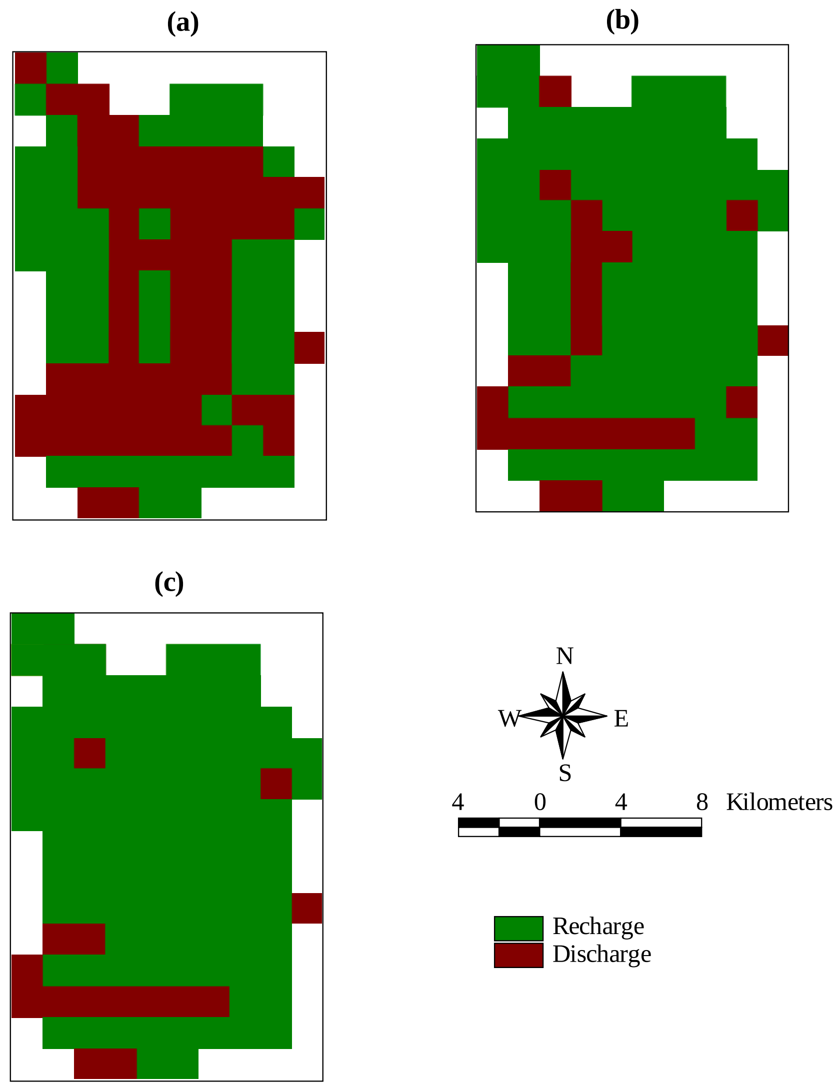


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